International consensus model for comparative assessment of chemical emissions in LCA

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Abstract

Under the UNEP-SETAC Life Cycle Initiative the six most commonly used characterization models for toxic impacts from chemicals were compared and harmonized through a sequence of workshops removing differences which were unintentional or unnecessary. A parsimonious (as simple as possible but as complex as needed) and transparent consensus model, USEtox, was created producing characterization factors that fall within the range of factors from the harmonised existing characterisation models. The USEtox model together with factors for several thousand substances are currently under review to form the basis of the recommendations from the UNEP-SETAC Life Cycle Initiative in this field.

Keywords

LCIA, chemicals, ecotoxicity, human toxicity, characterization modelling

1 INTRODUCTION

In Life Cycle Impact Assessment (LCIA) the emissions which occur in the life cycle of a product are translated (characterised) into their potential impacts on the environment ranging from local impacts from land use over regional impacts due to e.g. toxic substances, acidification or photochemical oxidants to global climate change. For each category of impact, the impact assessment applies substance-specific characterization factors (CFs) which represent the substance's potency. For most chemicals and release scenarios, there are not sufficient measurements to calculate CFs without the use of models. This places a demand on the community of LCIA scientists to develop and evaluate for this process models that are (a) sufficiently detailed to capture all the relevant elements, (b) transparent and easy to use, and (c) able to provide consistent and accurate results [1].

The purpose of this paper is to describe the approach and results of a model comparison and consensus building process for characterization modeling of human health and ecotoxicological impacts, which was initiated in 2003 and carried out by a Task Force of the joint Life Cycle Initiative of UNEP and SETAC [2].The process involved the model developers behind all the prominent characterization models worldwide, and was to both evaluate the differences among existing characterization models and to build consensus on good principles for characterization modeling. It has created a common understanding among the participants regarding which elements of the characterization models are the most important for the resulting characterization factors. Through harmonization of parameter choices in the participating models, differences among the calculated CFs for a given substance have been reduced substantially. Finally, a consensus model, USEtox, has been developed, which is supported by all participating model teams as a basis for future recommendations of characterization factors.

2 BACKGROUND

The Life Cycle Initiative was launched April 2002 as a collaboration between the United Nations Environment Program (UNEP) and the Society of Environmental Toxicology and Chemistry (SETAC) to "develop and disseminate practical tools for evaluating the opportunities, risks, and trade-offs associated with products and services over their entire life cycle to achieve sustainable development". An aim under the Initiative is to identify a recommendable practice for Life Cycle Assessment (LCA) within the framework laid out by the ISO standards ([3] [4]) and to make data and methodology for performing LCA available and applicable worldwide. For LCIA, this involves recommendation of specific characterization models and factors for the different categories of environmental impact, based on a global consensus process among experts, focusing on the scientific validity of the methods and their feasibility in LCIA [2]. Such a recommendation from UNEP-SETAC will meet the requirement of the ISO standard for Life Cycle Impact Assessment that "…the impact categories, category indicators and characterization models should be internationally accepted, i.e. based on an international agreement or approved by a competent international body" [4].

The Task Force on Toxic Impacts was established in 2003 under the LCIA branch of the Life Cycle Initiative as one of several task forces addressing the different categories of environmental impact normally included in an LCA[1].

[1] The UNEP-SETAC Task Force on Toxic Impacts had the following members: Bill Adams (USA), Till Bachmann (Germany), Cécile Bulle (Canada), Sau Soon Chen (Malaysia), Louise Deschênes (Canada), Evangelia Demou (Switzerland), Jeroen Guinée (Netherlands), Michael Hauschild (Denmark), Stefanie Hellweg (Switzerland), Mark Huijbregts (Netherlands), Olivier Jolliet (USA), Annette Köhler (Switzerland), Henrik Fred Larsen (Denmark), Manuele Margni (Canada), Tom McKone (USA), Dik van de Meent (Netherlands), Manuel Olivera (Colombia), Stig Irving Olsen (Denmark), Jérôme Payet (Switzerland), Pierre-Yves Robidoux (Canada), Ralph Rosenbaum (Switzerland), Andrea Russel (USA), Marta Schuhmacher (Spain).

An emission inventory for the life cycle of a product often contains hundreds of substances. It is estimated that 10-20 000 different chemicals are used in (the manufacture of) products marketed within the EU, for instance. Many of these substances have the potential to cause toxicity to humans or ecosystems when released to the environment and should thus have characterization factors for the human health and ecotoxicity categories of impact. A number of different models have been developed for this purpose around the world over the last 15 years (e.g. [5] [6] [7] [8] [9] [10] [11] [12] [13] [14]). The models vary substantially in their scope, applied modeling principles and not least in terms of the characterization factors they produce, as revealed by comparative studies (e.g. [15] [16]). The models mentioned above typically have characterization factors published for less than 400 substances, and the current situation for the LCA practitioner who wishes to include the chemical-related impacts in the impact assessment is thus that: (a) there will probably be many substances in the life cycle inventory for which no characterization factor is available from any of the models, (b) for some substances several of the models may have published characterization factors, but these often vary substantially between the models. The chemical-related impacts are hence often excluded from the LCIA which de facto reduces it to an energy impact assessment [1]. This unsatisfactory situation was the background on which the Task Force on Toxic Impacts defined its objectives as[2]:

1) Identification of good modeling practice for characterization modeling of ecotoxicity, human toxicity and related categories with direct effects on ecosystem health and human health
2) Harmonisation of existing models
3) Recommendation of characterisation model
4) Recommendation of characterisation factors and provision of these for many substances
5) Guidance on use of characterisation factors

3 PROCESS AND METHODS

The task force delegated subtasks to minor groups and coordinated the work of these and secured continuous progress through regular monthly or bimonthly conference calls and meetings in conjunction to the annual SETAC Europe and SETAC North America conferences. The work performed by the task force members was voluntary and unpaid, however the task force did obtain some funding to support a series of targeted workshops for comparing characterization models (see below)[3].

3.1 Survey of existing models

The work of the task force started with establishing the state of the art through a survey of existing characterization models for toxic impacts and a comparative review based on the available documentation of these. The survey covered the models mentioned in Table 1 and served for the later selection of models to be included in a comprehensive comparison of the performance of existing characterisation models ([17]).

[2] In addition to the work on human health impacts and ecotoxic impacts from emissions to the environment, the task force also has activities on modelling of indoor exposure. These activities will not be discussed further here.

[3] These sponsors are gratefully thanked for their contribution in the Acknowledgment section.

Table 1: Models included in the review of existing characterization models for human and/or ecotoxic impacts performed by the task force in the establishment of state of the art within the field (based on [17]).

Model name	Reference	Modeling approach
Fh-IUCT	[14]	Environmental key parameters
Ecopoints	[5]	Effect normalisation
EDIP97	[9]	Environmental key parameters
USES-LCA	[8]	Integrated multimedia model
CalTOX	[11]	Integrated multimedia model
IMPACT 2002	[6] [12]	Integrated multimedia model
GLOBOX	[18]	Integrated multimedia model
EPS 2000	[13]	Based on empirical data
Eco-indicator 99	[7]	Integrated multimedia model
Ecosense	[10]	Integrated multimedia model
OMNIITOX	[19]	Integrated multimedia model

3.2 Expert workshops

In parallel to the literature review, the task force worked on defining good modelling practice and developed criteria and preliminary guidelines focusing on the sub elements of fate-, exposure- and effect modelling. These criteria and guidelines were based on the learnings from the model review and experience gained with existing and widely used multimedia fate, exposure, and effect models, as well as recommendations from a sequence of workshops involving task force members as well as experts outside the task force.

A workshop in Lausanne, Switzerland in December 2003 primarily addressed fate modeling elements and the use of ecotoxicity test data to derive effect indicators [20]. A workshop in Apeldoorn, the Netherlands in April 2004 focused on identifying specific issues for fate-, exposure- and effect modeling of metals and established a research agenda for the characterization modeling of metal compounds [21]. A workshop in Portland, USA in November 2004 dealt with modeling of dose-response relationships and the preference of different measures of potency and severity in LCIA [22].

In addition, the work of the task force benefited from insights created in the model comparison effort organized by the Organization for Economic Cooperation and Development (OECD) expert group on persistence of chemicals and long-range transport potential (LRTP) of substances, particularly for the fate modeling guidelines and in the organization of a comparison of existing characterization models [23].

3.3 Comparison and harmonization of existing characterization models

The development of guidelines for good modelling practice led the task force to organise a comparison of the results of the existing characterisation models to help identify those elements and characteristics of the models which had the strongest influence on the model results, the characterisation factors. Those parts of the model which had the strongest influence were thus the natural focus of the guidelines under development.

The task force identified models (mainly characterization models in current use in LCIA) from Europe, North American and Asia and invited the groups behind them to participate in a model comparison. Five groups accepted the invitation to participate in the first model comparison workshop held on 5-6 May 2006 in Bilthoven, The Netherlands in conjunction with the SETAC Europe conference in The Hague. The goals of this first workshop were to

(a) compare the participating models regarding their structure and results in terms of characterization factors and
(b) identify crucial exposure and effect issues on which the presently available models differ.

Most prior efforts and recommendations for environmental multimedia models have had a strong focus on the fate component but less emphasis on exposure and human health impacts. Thus, a key goal of the model comparison was to fill in this gap.

The models which were invited to participate in the comparison workshop were: CalTOX, EcoSense, EDIP, IMPACT 2002, USES LCA, WATSON [24], BETR [25] EPS, LIME [26], and OMNIITOX (see Table 1). Among these the first six participated.

Preceding this workshop, the modelers were asked to describe and characterize their models in terms of a number of characteristic features and to run their models on a substance database to produce specified output (including characterization factors for human toxicity and ecotoxicity and central fate-, exposure-, and effect measures).

The substance database which was provided to all modelers contained the required input data for a collection of 76 substances which together covered all relevant combinations of substance properties like (bio)degradability, hydrophobicity, volatility and toxicity. This rather small set of substances was thus seen as representing most of the chemical universe.

An analysis team compared and processed the results prior to the workshop to formulate preliminary findings and help focus the workshop. During the workshop these findings were discussed in order to identify the most significant sources of differences in the results of the models and develop recommendations for harmonisation of the models to remove unnecessary causes of difference. The comparison of the models and the recommendations which were developed took the differences in the resulting characterisation factors as starting point to ensure the relevance. In this first comparison round, characterization factors differed by several orders of magnitude for some of the substances. All outliers are potentially important since each chemical in the substance database should be seen as representative of a large group of chemicals with a similar combination of properties. The comparison results thus pointed to the need for further assessment of model parameters.

After the Bilthoven workshop, the participating models were adapted by the modellers following recommendations developed at the workshop and rerun on the substances in the input database. The results were analysed using a similar approach at two following model comparison workshops in Paris early September 2006 and in Montreal early November 2006 with further modifications in-between, resulting in a harmonisation of the characterisation models in terms of parameter choices and a reduction in the variation between the models as shown in the Results and Discussion section below.

The fate and exposure behaviour of metals is fundamentally different from the organics in several central aspects. For example, a crucial role is played by speciation, biodegradation is not a relevant removal mechanism, and bioconcentration may be governed by active uptake mechanisms (see [27] [28]). This was pointed out at the Apeldoorn workshop, where it was acknowledged that more research is needed in order to develop a satisfactory characterization model for metal compounds [21]. At the workshops in Paris and Montreal, the model comparison was therefore focused on the characterization of organic substances.

3.4 Development of the Consensus Model USEtox

Following the inspiration from a recently concluded comparison of models for prediction of persistence and long-range transport potential performed under OECD [23], it was decided at the first model comparison workshop in Bilthoven to try to develop a consensus model on which future recommendations from UNEP/SETAC could be based, and:

- not aim for "best" modelling practice but rather "universally acceptable" modelling practice;
- recognise value in different approaches;
- develop the consensus model through reduction with the aim to create a model which is as strongly correlated to the other models in the comparison as the models are to each other.

The participating modellers decided in a joint effort to attempt to develop a consensus model with the following characteristics

- parsimonious (as simple a s possible, as complex as needed) containing only the model elements which were identified as the most influential in the comparison of the existing characterisation models;
- transparent and well documented;
- falling within the range of the existing characterisation models, i.e. not differing more from characterisation models in the comparison than these differ among themselves;
- endorsed by the modellers behind all participating models.

If successful, the consensus model would be the basis of the final recommendations of characterisation factors under the SETAC-UNEP Life Cycle Initiative.

The fate module of the consensus model was developed as a Level III multimedia model [29] consisting of two nested boxes, a continental scale nested within a global scale. Both boxes have two soil compartments, a freshwater and a marine compartment, and an air compartment. It was deemed essential for calculating the correct exposure of humans to have an urban air box nested within the continental air box (see Figure 1).

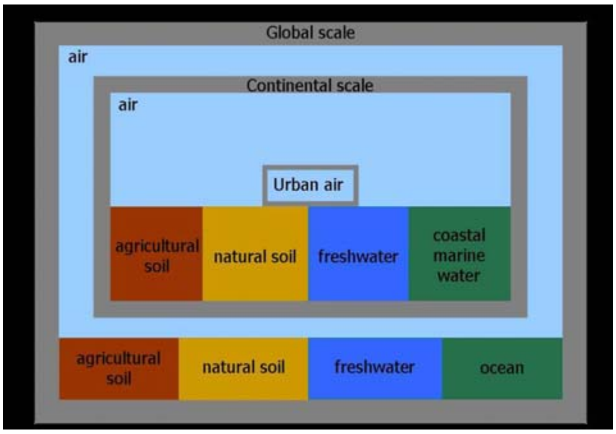

Figure 1: Box structure applied in the consensus model.

The consensus model was given the name USEtox (UNEP-SETAC toxicity model). The first prototype was developed after the first model comparison workshop in Bilthoven, and it entered the two following model comparison workshops in Paris and Montreal in parallel to the other models. It was continuously corrected and improved based on the outcome of the model comparisons to arrive at a version after the Montreal workshop, which showed satisfactory fit with the existing models (see Figure 2). This version has been submitted to an independent review by experts outside the model comparison process as part of the UNEP-SETAC endorsement of the model.

Pending the outcome of the review, the consensus model may be recommended for global use in LCIA of chemical emissions by the UNEP-SETAC International Life Cycle Panel in 2008 together with a database of recommended characterization factors for human toxicity (1200+ substances) and for ecotoxicity (2000+ substances) calculated using the model. Furthermore, interim factors are provided for ecotoxicity for an additional 2500+ substances for which the available data is insufficient to support a recommendation (but still judged better than nothing) or the model considered too uncertain to support a recommendation (metals and metal compounds).

4 RESULTS AND DISCUSSION

Through the model comparison, the existing characterization models were harmonized in their parameter choices as described earlier. This led to reductions in the differences between the characterization factors they produced as illustrated in Figure 2 showing two moments in time during the course of the work: plots of the characterization factors produced by a sub-set of the participating models against the factors from the USEtox model (a) at the first workshop in Bilthoven and (b) after the final workshop in Montreal. In addition to the factors shown in Figure 2, the models produce human health CFs for emissions to air, soil and water, and ecotoxicity CFs for emissions to air and water.

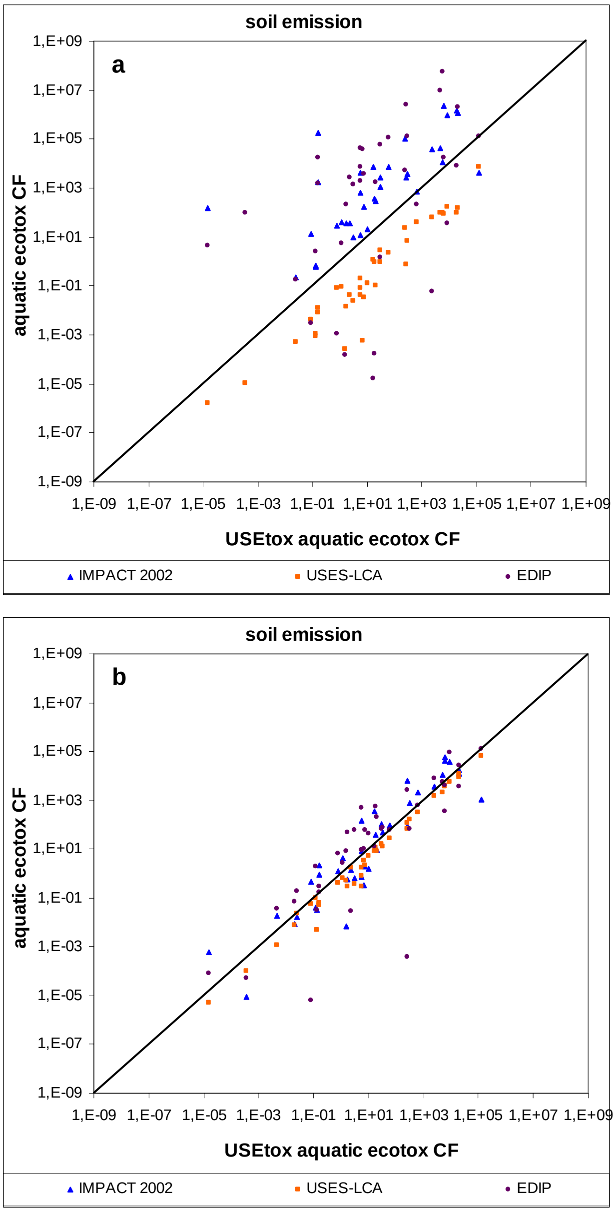

Figure 2: Aquatic ecotoxicity characterization factors for emission to soil of the substances in the short list (a) at the Bilthoven workshop and (b) after the Montreal workshop. All CFs expressed in the unit of the USEtox model (ecosystem health Comparative Toxicity Unit) through internal normalisation with a reference substance.

As seen from Figure 2 a and b, large reductions were achieved in the inter-model variability for the characterization factors for aquatic ecotoxic impacts from emissions to water. At the start, the variations between models typically spanned 5-8 and up to ten orders of magnitude, and after the third workshop this was reduced to two-three orders of magnitude difference for most substances.

Compared to what is known for other impact categories in LCIA (like global warming or eutrophication), 2-3 orders of magnitude variability between models is still a very large uncertainty since the choice of model is arbitrary – none of the models can be identified as more correct than the others. This inter-model variability should however be seen in the context of a variation of 10-12 orders of magnitude between the most and the least toxic substances for any model in the model comparison. In spite of the large uncertainty introduced by the choice of a specific characterization model, the characterization factors thus still enable us to discern between the substances and benchmark them according to their exposure and toxicity to humans or ecosystems.

In the analysis of differences between the models, particular attention was paid to individual outliers. As described earlier, the model comparison was based on a substance database with 76 substances selected with a view to represent the relevant combinations of substance properties. This approach implies that, in principle, every individual substance is important since it may represent a large group of substances with a similar combination of substance properties, and hence no outlier can be ignored a priori.

Another point of focus in the analysis was differences in 'slopes' between the models. Parallel clusters of substances typically represent scaling differences which are removed by calibration of the models, but differences in slopes indicate more fundamental modeling differences which need to be examined in more detail.

The USEtox model was developed with the explicit aim that the CFs it produces shall fall within the range of the existing characterisation models, i.e. the results of the consensus model must not differ more from the other characterisation models in the comparison than they differ from each other. Figure 2b shows that for the characterisation of aquatic ecotoxic impacts from soil emissions, this aim has been met by the developed model - the USEtox model has been used as reference model, and the factors from the other characterisation models are grouped around the factors of the USEtox model with no apparent bias. Similar results were obtained for other emission compartments and for human health impacts.

5 CONCLUSION AND OUTLOOK

The model comparison and the lessons learned from the process resulted in the development of a consensus model, USEtox, which is collectively endorsed by the Task Force and model providers, and presented as recommended practice. The USEtox model was developed with the aim of parsimony – as simple as possible and as complex as needed. It falls within the range of the existing characterisation models which participated in the model comparison for non-dissociating organic substances in the test set of chemicals, which was applied in the comparison, even after the existing characterisation models were harmonised to remove unintentional and unwanted differences. The model thus does not deviate more from the existing characterisation models than these deviate among each other.

USEtox has been used to calculate recommended characterization factors for 1200+ substances for human toxicity and 2000+ substances for ecotoxicity. In addition, interim factors have been calculated for substances for which the substance groups for which the model is not considered mature for a proper recommendation (such as dissociating organic substances, metals and inorganic substances). However, interim factors for these substances are still considered better than no factor at all. In the latter case, the assumption will often inherently be that the CF is zero. Overall, the substance coverage of USEtox is better than for any other characterisation model published until this day.

The characterization factors will have a limited period of validity. Better information about the substance's properties will become available and the USEtox model is also foreseen to undergo future updates as models become better. Updates will probably be preceded by new model comparison projects to ensure that USEtox remains representative of state-of-the-science characterisation models.

Foreseen next steps with the existing version of USEtox are a further development of the model to calculate better characterization factors for metals and inorganic substances. Work is also on-going to support inclusion of indoor exposure in the fate module of the model. It is acknowledged that indoor exposure takes place, and it may be orders of magnitude higher than the direct exposure to the same chemicals through the external environment.

The USEtox model currently exists as a spreadsheet model but programming in a more user-friendly software package is planned.

Additional information about the USEtox model will be uploaded to the model web-site: www.usetox.org.

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